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PERTURBATION THEORY AND SENSITIVITY ANALYSIS FOR TWO-DIMENSIONAL SHIELDING CALCULATIONS†

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ABSTRACT

The purpose of this work is to describe the development and implementation of perturbation theory methods for two-dimensional shielding problems. Cross section sensitivity results are obtained by calculating the effect of varying each individual cross section parameter.

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Changes in a response, R, can be calculated using the perturbation theory relationship[1]

$$\Delta R \simeq \iiint \phi^*(\bar{r},E,\bar{\Omega}) \left[\iint \delta\Sigma_s(\bar{r},E'\to E,\bar{\Omega}'\to\bar{\Omega}) \times\phi(\bar{r},E',\bar{\Omega}')\,dE'\,d\bar{\Omega}' - \delta\Sigma_t(\bar{r},E)\,\phi(\bar{r},E,\bar{\Omega}) \right] dE\,d\bar{\Omega}\,d\bar{r}, \tag{1}$$

where the perturbation is represented by the changes in the total and scattering cross sections and ϕ and ϕ^* are the forward and adjoint fluxes. This paper will deal with the evaluation of the above equation with forward and adjoint fluxes calculated using the discrete ordinates computer program DOT.[2] The spatial and energy integrations are easily evaluated by replacing the integrals with summations over energy groups and a space mesh. The angular integrations are more complicated and will be considered in more detail.

The scattering term in Equation (1) requires the evaluation of an integral of the form

$$\int_{4\pi} \phi^*(\bar{\Omega}) \int_{4\pi} \phi(\bar{\Omega}')\,\sigma(\bar{\Omega}\cdot\bar{\Omega}')\,d\bar{\Omega}'\,d\bar{\Omega}.$$

The cross section may be expanded in a Legendre series as

$$\sigma(\bar{\Omega}\cdot\bar{\Omega}') = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \sigma_\ell P_\ell(\bar{\Omega}\cdot\bar{\Omega}'), \tag{2}$$

where $\sigma_\ell = (2\ell+1) \int_{4\pi} \sigma(\bar{\Omega}\cdot\bar{\Omega}')P_\ell(\bar{\Omega}\cdot\bar{\Omega}')\,d\bar{\Omega}$. Similarly, the angular fluxes may be expanded in a spherical harmonic series as

$$\phi(\bar{\Omega}) = \sum_{\ell=0}^{\infty} \sum_{m=0}^{\ell} \frac{2\ell+1}{4\pi}\, j_{\ell,m}\, A_\ell^m(\bar{\Omega}), \tag{3}$$

and

$$\phi^*(\bar{\Omega}) = \sum_{\ell=0}^{\infty} \sum_{m=0}^{\ell} (-1)^\ell (2\ell+1)\, j^*_{\ell,m}\, A_\ell^m(\bar{\Omega}), \tag{4}$$

where

$$j_{\ell,m} = \int_{4\pi} \phi(\bar{\Omega}) A_\ell^m(\bar{\Omega})\, d\bar{\Omega},$$

$$j^*_{\ell,m} = \frac{1}{4\pi} \int_{4\pi} \phi^*(-\bar{\Omega}) A_\ell^m(\bar{\Omega})\, d\bar{\Omega},$$

$$A_\ell^m(\bar{\Omega}) = \left(\frac{2}{1+\delta_{0,m}} \frac{(\ell-m)!}{(\ell+m)!}\right)^{1/2} P_\ell^m(\eta) \cos m\psi,$$

$$\int_{4\pi} d\bar{\Omega} = \int_0^{2\pi} \int_{-1}^{1} d\eta\, d\psi,$$

and

$$A_\ell^m(-\bar{\Omega}) = (-1)^\ell A_\ell^m(\bar{\Omega}).$$

The form of the above equations was chosen to conform with the equations programmed in DOT. The $(-1)^\ell$ and $-\bar{\Omega}$ factors arise because the adjoint problem is solved for $\phi^*(-\bar{\Omega})$.

The addition theorem for legendre polynomials is (ignoring terms that vanish under integration):

$$P_\ell(\bar{\Omega}\cdot\bar{\Omega}') = \sum_{m=0}^{\ell} A_\ell^m(\bar{\Omega}) A_\ell^m(\bar{\Omega}'). \tag{5}$$

Substitution of Equations (2), (3), (4), and (5) into the desired integral and use of the orthogonality relationship,

$$\int_{4\pi} A_\ell^m(\bar{\Omega}) A_{\ell'}^{m'}(\bar{\Omega})\, d\bar{\Omega} = \frac{4\pi}{2\ell+1} \delta_{\ell,\ell'} \delta_{m,m'}, \tag{6}$$

yields the final result:

$$\int_{4\pi} \phi^*(\bar{\Omega}) \int_{4\pi} \phi(\bar{\Omega}') \sigma(\bar{\Omega}\cdot\bar{\Omega}')\, d\bar{\Omega}'\, d\bar{\Omega} = \sum_{\ell=0}^{\infty} \sum_{m=0}^{\ell} (-1)^\ell \sigma_\ell j_{\ell,m} j^*_{\ell,m}. \tag{7}$$

The total cross section term in Equation (1) requires the evaluation of an integral of the form

$$\int_{4\pi} \phi(\bar{\Omega}) \phi^*(\bar{\Omega})\, d\bar{\Omega}.$$

This integral can be evaluated using the angular fluxes from the discrete ordinates calculation as has been done in one-dimensional calculations.[3,4] However, because of the tremendous quantity of numbers to be stored in two-dimensional problems (70 million for the example which follows), it is highly desirable to avoid storing the angular flux if possible. A way to avoid the angular flux may be found by substituting Equations (3) and (4) into the desired integral and using Equation (6) to obtain

$$\int_{4\pi} \phi(\bar{\Omega})\phi^*(\bar{\Omega})\,d\bar{\Omega} = \sum_{\ell=0}^{\infty}\sum_{m=0}^{\ell} (-1)^{\ell}(2\ell+1)j_{\ell,m}j^*_{\ell,m}. \qquad (8)$$

Thus, Equation (1) can be evaluated using only the flux moments $j_{\ell,m}$ and $j^*_{\ell,m}$ provided the series in Equations (7) and (8) can be truncated after a few terms without serious error. Present experience indicates that a third order expansion (through $\ell=3$) is sufficient for many problems.

The approach outlined above has been implemented using the computer programs VIP[5] and SWANLAKE[6]. The method was tested for a deep penetration sodium problem and for an infinite air calculation (including a first collision source term) by comparing with 1-D SWANLAKE calculations. Agreement was satisfactory in both cases.

The first realistic two-dimensional sensitivity analysis performed in this study was for the calculation of neutron and gamma doses at the maintenance deck of the FTR.[7] The DOT calculations were performed with a 21-18 coupled neutron-gamma ray cross section set, a 166 angle quadrature set suitable for streaming in annular gaps, and P_3 scattering.

Results obtained from the sensitivity analysis include the sensitivity of neutron and gamma dose to changes in cross sections as a function of position, energy, and element. For this problem, the important gamma ray sources are iron (n,γ) reactions (primarily in the stainless steel head) which are responsible for 55 percent of the gamma dose and boron (n,γ) reactions (in a borated polyethylene layer under the maintenance deck) which contributes 28 percent of the gamma dose. A more detailed study indicates that 31 percent of the gamma dose is due to gamma ray production in the 7 to 8 MeV group, which contains strong iron (n,γ) production lines at 7.63 and 7.65 MeV. The gamma dose due to boron production is the result of the (n,γ) 0.48 MeV line.

This work demonstrates the feasibility of performing sensitivity studies and perturbation calculations for two-dimensional shielding problems. The FTR example shows the usefulness of calculations of this type for realistic shielding applications.

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